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                CASREACT(R) - Over 10 million reactions available
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                2006 MeSH terms loaded in MEDLINE/LMEDLINE
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                2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
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        DEC 14
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                CA/CAplus to be enhanced with updated IPC codes
NEWS
     7
        DEC 21
                IPC search and display fields enhanced in CA/CAplus with the
                IPC reform
NEWS 8
        DEC 23
               New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
                USPAT2
NEWS 9
        JAN 13
                IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 10 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                INPADOC
NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV
NEWS 13 JAN 30 Saved answer limit increased
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency
                added to TULSA
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NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
http://download.cas.org/express/v8.0-Discover/

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=> FILE REG COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 02:07:50 ON 06 FEB 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 FEB 2006 HIGHEST RN 873528-70-2 DICTIONARY FILE UPDATES: 3 FEB 2006 HIGHEST RN 873528-70-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

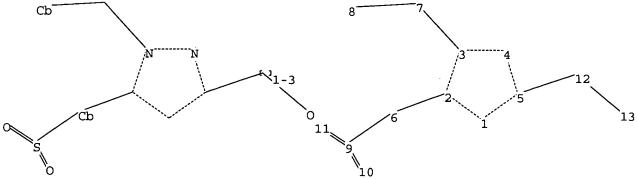
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10628375.str



Page 2

chain nodes :

6 7 8 9 10 11 12 13

ring nodes : 1 2 3 4 5 chain bonds :

2-6 3-7 5-12 6-9 7-8 9-10 9-11 12-13

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-7 4-5 9-10 9-11 12-13

exact bonds:
2-6 5-12 6-9 7-8
isolated ring systems:
containing 1:

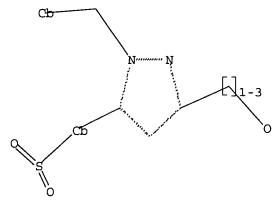
J

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS

## L1 STRUCTURE UPLOADED

=> D L1 HAS NO ANSWERS L1 STE



Structure attributes must be viewed using STN Express query preparation.

=> S L1

SAMPLE SEARCH INITIATED 02:08:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 541 TO ITERATE

100.0% PROCESSED 541 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 9425 TO 12215

PROJECTED ANSWERS: 0 TO 0

Page 3 saeed

L2 0 SEA SSS SAM L1

=> S L1 FULL

FULL SEARCH INITIATED 02:08:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10476 TO ITERATE

100.0% PROCESSED 10476 ITERATIONS

14 ANSWERS

SEARCH TIME: 00.00.01

L3 14 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

166.94 167.15

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FILE COVERS 1907 - 6 Feb 2006 VOL 144 ISS 7 FILE LAST UPDATED: 5 Feb 2006 (20060205/ED)

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=> S L3

L4 3 L3

=> D IBIB ABS HITSTR TOT

L4 ANSWER 1 OF 3
ACCESSION NUMBER:
DOCUMENT NUMBER:
DOCUMENT NUMBER:
DOCUMENT NUMBER:
SYNTHESIS and Selective Cyclooxygenase-2 Inhibitory
Activity of a Series of Novel, Nitric Oxide
Donor-Containing Pyrazoles
AUTHOR(S):

A

Journal

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): English CASREACT 140:423618

The synthesis of a series of novel pyrazoles containing a nitrate (ONO2) moiety as a nitric oxide (NO)-donor functionality is reported. Their COX-1 and COX-2 inhibitory activities in human whole blood are profiled. The data demonstrate that pyrazole ring substituents play an important role in COX-2 selective inhibition, such that a cycloalkylpyrazole (1, X = CH2) was found to be a potent and selective COX-2 inhibitor. Other modifications at the 3 position of the central pyrazole ring (I, X = CG103), (10NH) (CH2)3, (2)-CH1CGH2CH2) enhanced COX-2 inhibitory potency. Among the pyrazoles synthesized, the oxine [I, X = CG1001] (CH2)3] was identified as the most potent COX-2 selective inhibitor. Accordingly, this compound was profiled pharmacol: in the rat after oral administration and shown to possess potent antifoliamatory activity in the carrageenan-induced air-pouch model and less gastric toxicity than a dard AB

carrageenan-induced air-pouch model and less yastize towarts, came a standard cOX-2 inhibitor when administered with background aspirin treatment. The enhanced gastric tolerance of an No-donor COX-2 selective inhibitor has the potential to augment the clin. profile of this drug class.

If 634058-48-7P 634058-51-2P 634058-53-4P RI: PRC (Pharmacological activity), RCT (Reactant), SPN (Synthetic preparation), BIOL (Biological study), PREP (Preparation), RACT (Reactant

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) or reagent)
(prepn. and selective cyclooxygenase-2 inhibitory activity of nitric oxide donor-contg. pyrazoles)
654058-48-7 CAPLUS
H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-(9CI) (CA INDEX NAME)

654058-51-2 CAPLUS
1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-(9C1) (CA INDEX NAME)

654058-53-4 CAPLUS
IR-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-(SCI) (CA INDEX NAME)

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



— (CH2) 3 но

654058-52-3P 654058-60-3P 654058-64-7P
654058-66-9P 654058-67-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREF (Preparation)
(preparation and selective cyclooxygenase-2 inhibitory activity of nitric oxide donor-containing pyrazoles)
654058-52-3 CAPLUS
2-Propen-1-01, 3-{1-(cyclohexylmethyl)-5-(4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

654058-60-3 CAPLUS
1H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl)nitrate (ester) (SCI) (CA INDEX NAME)

654058-64-7 CAPLUS

Page 5

saeed

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1H-Pyrazole-3-methanol, 5-(4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, nitrate (ester) (SCI) (CA INDEX NAME)

654058-66-9 CAPLUS
2-Propen-1-01, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1Hpyrazol-3-yl]-, nitrate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

654058-67-0 CAPLUS
1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl], nitrate (ester) (9C1) (CA INDEX NAME)

02N-0- (CH2) 3

REFERENCE COUNT:

THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:100955 CAPLUS
DOCUMENT NUMBER: 10:157441
TITLE: Cycloxygenase- 2 selective inhibitors, compositions and methods of use
Garvey, David S.; Khanapure, Subhash P.; Ranatunge, Ramani R.; Richardson, Stewart K.; Schroeder, Joseph

PATENT ASSIGNEE(S): SOURCE:

D.
Nitromed, Inc., USA
PCT Int. Appl., 140 pp.
CODEN: PIXXD2 DOCUMENT TYPE:

Patent English 1 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	ENT I						DATE									ATE	
	2004						2004						605			0030	
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CA	2493	156			AA		2004	0205		CA 2	003-	2493	156		2	0030	729
US	2004	0728	83		A1		2004	0415	1	US 2	003-	6283	75		2	0030	729
EP	1542	972			A2		2005	0622		EP 2	003-	7720	04		2	0030	729
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ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

654058-53-4 CAPLUS 1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl](9CI) (CA INDEX NAME)

HO- (CH2) 3

654058-67-0 CAPLUS

1H-Pyrazole-3-propanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (9CI) (CA INDEX NAME)

02N-0- (CH2)3

654058-56-7P 654058-58-9P 654058-60-3P 654058-62-3P 654058-64-7P RE: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES

(antiinflammatory cyclooxygenase-2 selective inhibitors)

RN 654058-56-7 CAPLUS
CN 2-Propencic acid, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl}-1H-

Page 6 saeed

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) improving the cardiovascular profile of COX-2 selective inhibitors. 654058-48-79 654058-51-29 654058-52-39 654058-53-49 654058-67-09 RE: FAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (antiinflammatory cyclocxygenase-2 selective inhibitors) 654058-48-7 CAPLUS (H-Pyrazole-3-methanol, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-(9CI) (CA INDEX NAME)

654058-51-2 CAPLUS IH-Pyrazole-3-mathanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-(SCI) (CA INDEX NAME)

654058-52-3 CAPLUS 2-Propen-1-ol, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) pyrazol-3-yl)-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

654058-58-9 CAPLUS
1H-Pyrazole-3-carboxylic acid, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)

654058-60-3 CAPLUS | 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, nitrate (ester) (SCI) (CA INDEX NAME)

02N-0-CH2

654058-62-5 CAPLUS Ethanol, 2-([1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]methoxyl-, nitrate (ester) (SCI) (CA INDEX NAME)

## L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

654058-64-7 CAPLUS
1H-Pyrazole-3-methanol, 5-[4-(methylsulfonyl)phenyl]-1-(phenylmethyl)-, nitrate (ester) (SCI) (CA INDEX NAME)

ΙŤ

654058-66-9

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antiinflammatory cyclooxygenase-2 selective inhibitors)
654058-66-9 CAPUS
2-Propen-1-01, 3-[1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-1H-pyrazol-3-yl]-, nitrate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

## 654058-86-32

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER:
DOCUMENT NUMBER:
1111E:
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111IE:
11IIIE:
11II

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9925695	A1	19990527	WO 1998-JP5041	19981110
W: JP, US				
RW: AT, BE, CH,	CY, DE,	DK, ES,	FI, FR, GB, GR, IE,	IT, LU, MC, NL,
PT, SE				
JP 2002509554	T2	20020326	JP 1999-528127	19981110
RIORITY APPLN. INFO.:			AU 1997-423	A 19971118
			WO 1998-JP5041	W 19981110
THER SOURCE (S):	MARPAT	131:5254		

The title compds. [I; Rl = (un)substituted aryl; R2 = H, NH2, halo, etc.; R3 = H, aryl optionally substituted with halogen, lower alkyl; R4 = (un)substituted aryl; A = lower alkylene], useful for the treatment and/or prevention of inflammatory conditions, various pains, collagen diseases, autoimmune diseases, various immunity disease, analgesic, thrombosis, cancer or neurodegenerative diseases, were prepared Thus; refluxing 4,4,4-trifluoro-1-[4-(methylsulfonyl)phenyl]butane-1,3-dione with 3-fluorobensylhydrazine in AcOH afforded I [A = CH2; Rl = 3-FCGH4; R2 = CF3; R3 = H; R5 = 4-(MeSO2)CGH4] which showed secondary lesion inhibition (uninjected paw) of > 60% at 1.0 mg/kg in rats.
225791-84-09; 225791-90-89
RL: RAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of 5-arylpyrazoles as COX-2 selective inhibitors) 225791-84-0 CAPLUS (BLOGGEN); CA INDEX NAME)

Page 7 saeed ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continu (Reactant or reagent) (antininflammatory cyclooxygenase-2 selective inhibitors) 654058-86-3 CAPLUS H-Pyrazole-3-carboxylic acid, 1-(cyclohexylmethyl)-5-[4-(methylsulfonyl)phenyl]-, methyl ester (9CI) (CA INDEX NAME) (Continued)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

225781-90-8 CAPLUS
1H-Pyrazole-3-carboxylic acid, 1-{(2,4-difluorophenyl)methyl}-5-{4-(methylsulfonyl)phenyl}-, ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

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COST IN U.S. DOLLARS TOTAL SESSION SINCE FILE ENTRY

FULL ESTIMATED COST 16.25 183.40

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ENTRY SESSION -2.25 CA SUBSCRIBER PRICE

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